



Workshop Report Schedule

**Large Scale Computing and Storage Requirements
for Basic Energy Sciences Research**

Joint BES / ASCR / NERSC Workshop

February 9-10, 2010



Logistics: Final Report Content

- Overview
 - Executive Summary (NERSC writes)
 - Findings (NERSC)
 - NERSC Response
- BES Goals (DOE writes)
- Chemistry, Materials, Geosciences goals
- Case studies: specific examples
 - What scientific questions will be addressed
 - What's needed from NERSC to do so



Logistics: Final Report Content

- Key element of case studies: how science goals drive NERSC requirements
 - Want a direct relationship between *specific* science goals and NERSC needs
 - “In 3 years we want to be able to study 'X' but to do so requires '1,2,3' ”
 - Or “Having access to 50x resources will allow us to resolve 'X' or understand 'Y' ”
 - Etc.

Input

- Basically 3 inputs
 - The worksheet you filled out already;
 - The case study template and examples from previous NERSC BER workshop;
 - Other considerations that came up during discussions on Tuesday and Wednesday
 - Either full-group or during science area telecons



Logistics: Final Report Schedule

- Case studies due to NERSC: **March 8**
- NERSC draft report: April 2
- Participants review period: **April 2-16**
- NERSC Near final: April 30
- BER AD approval: May 7
- NERSC Revisions: May 21
- Final Report posted: June 4

Important participant deadlines in red



Examples of Information Sought

- Type of simulation, #, reason for #, algorithms, solver
- Parallelism: method, weak or strong scaling, implementation, concurrency, limits
- Key physical parameters and their limits:
 - spatial resolution, # of atoms/energy levels, integration range, ...
- Representative code
- Key science result metrics and goals



Examples of Information Sought

- Typical science process (workflow)
- Data: amount stored / transferred for input, results, and fault mitigation
- Special needs for data intensive projects
 - Grids, gateways, workflows, provenance, `
- Special query regarding multicore/manycore
- How all of this is
 - Driven by the science
 - Likely to change and why

Scaling Science

Inspired by **P. Kent**,
“*Computational Challenges in
Nanoscience: an ab initio
Perspective*”, Peta08 workshop,
Hawaii (2008) and **Jonathan
Carter** (NERSC).

**Convergence,
systematic errors
due to cutoffs, etc.**

**Length, Spatial
extent, #Atoms, *Weak
scaling***

**Time scale
Optimizations, *Strong
scaling***

**Initial Conditions, e.g.
molecule,
boundaries,
*Ensembles***

**Simulation method,
e.g. DFT, QMC or HF/
SCF; LES or DNS**